

=> fil hcaplus
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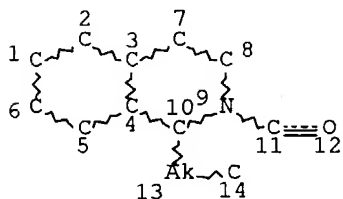
FILE COVERS 1907 - 31 Aug 2004 VOL 141 ISS 10
 FILE LAST UPDATED: 30 Aug 2004 (20040830/ED)

This file contains CAS Registry Numbers for easy and accurate substance identification.

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=> d stat que
 L3 STR



NODE ATTRIBUTES:

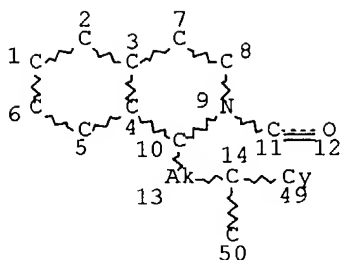
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 DEFAULT MLEVEL IS ATOM
 DEFAULT ECLEVEL IS LIMITED

GRAPH ATTRIBUTES:

RING(S) ARE ISOLATED OR EMBEDDED
 NUMBER OF NODES IS 14

STEREO ATTRIBUTES: NONE

L5 3465 SEA FILE=REGISTRY SSS FUL L3
 L20 STR



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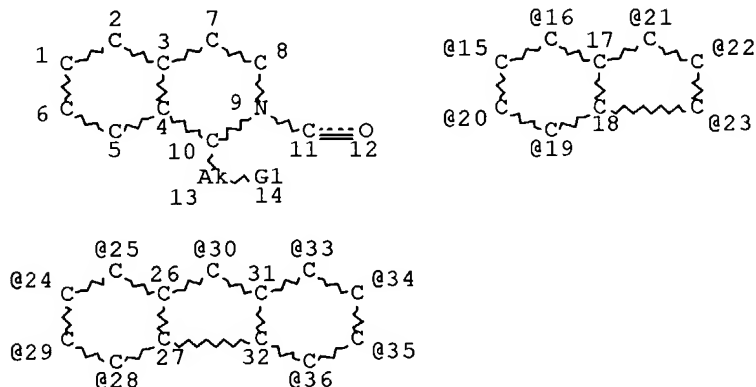
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 DEFAULT ECLEVEL IS LIMITED

GRAPH ATTRIBUTES:

RING(S) ARE ISOLATED OR EMBEDDED
 NUMBER OF NODES IS 16

STEREO ATTRIBUTES: NONE

L21 5 SEA FILE=REGISTRY SUB=L5 SSS FUL L20
 L22 STR



VAR G1=15/16/21/22/23/19/20/24/25/30/28/29/33/34/35/36

NODE ATTRIBUTES:

DEFAULT MLEVEL IS ATOM
 DEFAULT ECLEVEL IS LIMITED

GRAPH ATTRIBUTES:

RING(S) ARE ISOLATED OR EMBEDDED
 NUMBER OF NODES IS 36

STEREO ATTRIBUTES: NONE

L23 0 SEA FILE=REGISTRY SUB=L5 SSS FUL L22
 L24 5 SEA FILE=REGISTRY ABB=ON PLU=ON (L21 OR L23)
 L25 4 SEA FILE=HCAPLUS ABB=ON PLU=ON L24

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=>

=> d ibib abs hitstr l25 1-4

L25 ANSWER 1 OF 4 HCAPLUS COPYRIGHT 2004 ACS on STN

ACCESSION NUMBER: 1996:335639 HCAPLUS Full-text

DOCUMENT NUMBER: 125:58291

TITLE: Reaction of 3,4-dihydroisoquinolines with
1,3-dicarbonyl compounds and carboxylic acid
chlorides. Novel synthesis of 2-(2-
acyltetrahydroisoquinolin-1-yl)-1,3-dicarbonyl
compounds

AUTHOR(S): Akhrem, A. A.; Borisov, E. V.; Chernov, Yu. G.

CORPORATE SOURCE: Inst. Bioorg. Khim., Akad. Nauk Respub. Belarus,
Minsk, Belarus

SOURCE: Zhurnal Organicheskoi Khimii (1995), 31(11), 1715-1720
CODEN: ZORKAE; ISSN: 0514-7492

PUBLISHER: Nauka

DOCUMENT TYPE: Journal

LANGUAGE: Russian

AB Reaction of 3,4-dihydroisoquinolines with carboxylic acid chlorides and 1,3-
dicarbonyl compds. (1,3-diketones and β -keto esters) produced a series of 2-(2-
acyltetrahydroisoquinolin-1-yl)-1,3-dicarbonyl compds. The stereochem. and
tautomerism of the products were discussed.

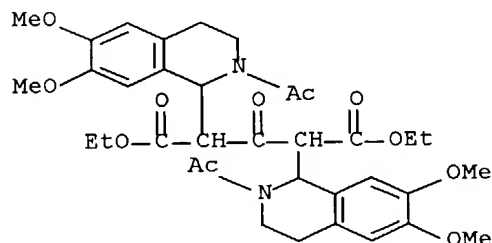
IT **175983-15-0P 175983-16-1P**

RL: SPN (Synthetic preparation); PREP (Preparation)

(preparation of 2-(2-acyltetrahydroisoquinolin-1-yl)-1,3-dicarbonyl compds.
by reaction of 3,4-dihydroisoquinolines with 1,3-dicarbonyl compds. and
carboxylic acid chlorides)

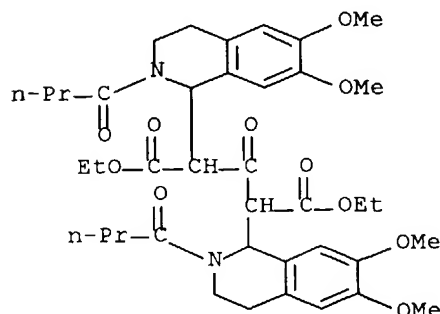
RN 175983-15-0 HCAPLUS

CN Pentanedioic acid, 2,4-bis(2-acetyl-1,2,3,4-tetrahydro-6,7-dimethoxy-1-
isoquinolinyl)-3-oxo-, diethyl ester (9CI) (CA INDEX NAME)

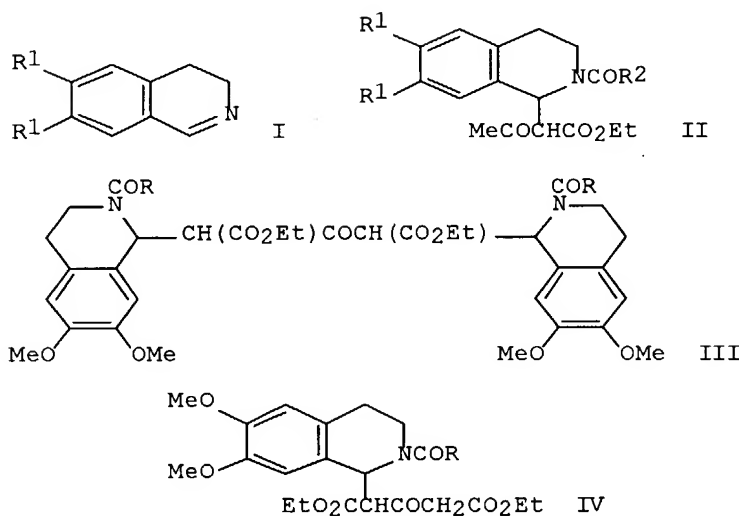


RN 175983-16-1 HCAPLUS

CN Pentanedioic acid, 3-oxo-2,4-bis[1,2,3,4-tetrahydro-6,7-dimethoxy-2-(1-
oxobutyl)-1-isoquinolinyl]-, diethyl ester (9CI) (CA INDEX NAME)



L25 ANSWER 2 OF 4 HCAPLUS COPYRIGHT 2004 ACS on STN
ACCESSION NUMBER: 1996:162169 HCAPLUS Full-text
DOCUMENT NUMBER: 124:316960
TITLE: Reaction of 3,4-dihydroisoquinolines with β -keto
ester enol acylates
AUTHOR(S): Akhrem, A. A.; Borisov, E. V.; Chernov, Yu. G.
CORPORATE SOURCE: Inst. Bioorg. Khim., Minsk, Belarus
SOURCE: Zhurnal Organicheskoi Khimii (1995), 31(8), 1241-5
CODEN: ZORKAE; ISSN: 0514-7492
PUBLISHER: Nauka
DOCUMENT TYPE: Journal
LANGUAGE: Russian
GI



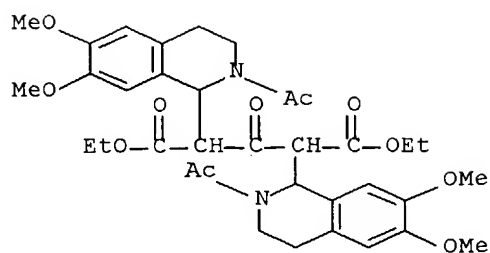
AB Dihydroisoquinolines I (R1 = H, MeO) reacted with R2CO2CMe:CHCO2Et (R2 = Ph, Me) to give adducts II. I (R1 = MeO) reacted with EtO2CCH2C(OCOR):CHCO2Et (R = Me, Pr) to give adducts III and IV.

IT 175983-15-0P 175983-16-1P

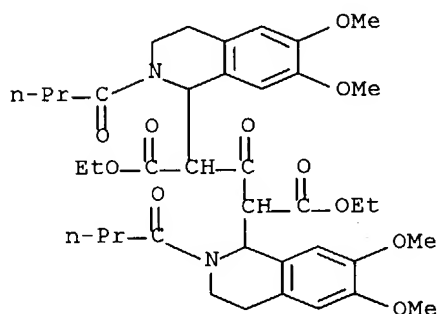
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation of)

RN 175983-15-0 HCAPLUS

CN Pentanedioic acid, 2,4-bis(2-acetyl-1,2,3,4-tetrahydro-6,7-dimethoxy-1-isoquinoliny1)-3-oxo-, diethyl ester (9CI) (CA INDEX NAME)



RN 175983-16-1 HCAPLUS
 CN Pentanedioic acid, 3-oxo-2,4-bis[1,2,3,4-tetrahydro-6,7-dimethoxy-2-(1-oxobutyl)-1-isoquinolinyl]-, diethyl ester (9CI) (CA INDEX NAME)



L25 ANSWER 3 OF 4 HCAPLUS COPYRIGHT 2004 ACS on STN
 ACCESSION NUMBER: 1967:516903 HCAPLUS Full-text
 DOCUMENT NUMBER: 67:116903
 TITLE: Reaction of vinyl bromide and substituted vinyl bromides with lithium in tetrahydrofuran with formation of lithium acetylides
 AUTHOR(S): Schoepf, Clemens; Strauss, Hans J.; Hoehn, Monika; Hutzler, Anneliese
 CORPORATE SOURCE: Tech. Hochsch., Darmstadt, Fed. Rep. Ger.
 SOURCE: Monatshefte fuer Chemie (1967), 98(4), 1274-309
 CODEN: MOCHAP
 DOCUMENT TYPE: Journal
 LANGUAGE: German

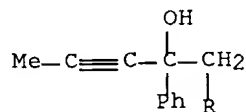
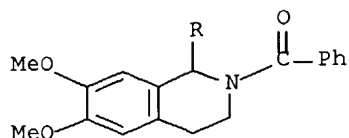
AB Treatment of 2-bromopropene and 2-bromo-1-butene with Li in boiling tetrahydrofuran (THF) led to Li acetylides, instead of the expected Li alkenes. The major products were the free alkene and LiBr, with a smaller amount of LiH. Similarly, with vinyl bromide the acetylide was formed together with LiH, while Li vinyl was not found. cis-1-Bromo-1-butene also gave the acetylide. In THF the formation of Li acetylide from 2-bromopropene proceeded at -65°, while in Et2O reflux temps. were required. Acetylides were also obtained from PhC.tplbond.CH and 1-octyne, while very little reaction was observed with HC.tplbond.CH. The mechanism of acetylide formation is discussed.

IT **16557-12-3P 16557-17-8P**

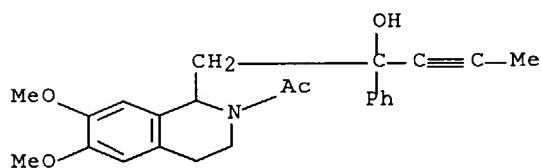
RL: SPN (Synthetic preparation); PREP (Preparation)
 (preparation of)

RN 16557-12-3 HCAPLUS

CN 1-Isoquinolineethanol, 2-benzoyl-1,2,3,4-tetrahydro-6,7-dimethoxy-α-phenyl-α-1-propynyl- (8CI) (CA INDEX NAME)



RN 16557-17-8 HCAPLUS

CN 1-Isoquinolineethanol, 2-acetyl-1,2,3,4-tetrahydro-6,7-dimethoxy- α -phenyl- α -1-propynyl- (8CI) (CA INDEX NAME)

L25 ANSWER 4 OF 4 HCAPLUS COPYRIGHT 2004 ACS on STN
 ACCESSION NUMBER: 1964:418195 HCAPLUS Full-text
 DOCUMENT NUMBER: 61:18195
 ORIGINAL REFERENCE NO.: 61:3079h,3080a-h
 TITLE: Quinolizine derivatives
 INVENTOR(S): Schoepf, Clemens; Klug, Rudolf
 PATENT ASSIGNEE(S): E. Merck, A.G.
 SOURCE: 8 pp.
 DOCUMENT TYPE: Patent
 LANGUAGE: Unavailable
 PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
US 3132147		19640505	US	
BE 632428			BE	
FR 1431659			FR	
GB 977725			GB	

PRIORITY APPLN. INFO.: DE 19610619

OTHER SOURCE(S): CASREACT 61:18195

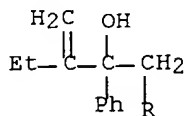
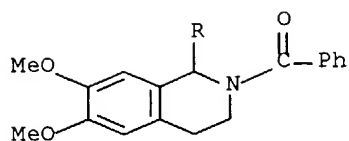
GI For diagram(s), see printed CA Issue.

AB Vinyl bromide (105 g.) in 240 ml. tetrahydrofuran (THF) is treated with 24 g. Mg. in 210 ml. THF to form the Grignard compound, an addnl. 350 ml. THF added, 60 g. 1-phenacyl-6,7-dimethoxy-1,2,3,4-tetrahydroisoquinoline added with stirring and cooling, the mixture kept at 35° 4.5 hrs. and decomposed with ice-cooling with 250 ml. of saturated NH₄Cl, the THF layer separated, and the residue extracted with CH₂Cl₂ to give, from the combined organic solvents, 68% [(6,7-dimethoxy-1,2,3,4-tetrahydro-1-isoquinolyl)methyl](phenyl)(vinyl)carbinol (I), m. 126-8° (iso-PrOH); HCl salt m. 210-12° (EtOH); HBr salt m. 215-16° (EtOH). A solution of 14.8 g. I.HCl in 61 ml. SOCl₂ is kept at room temperature 16 hrs. and the SOCl₂

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evaporated to yield 62.6% 1-(6,7-dimethoxy-1,2,3,4-tetrahydro-1-isoquinolyl)-2-phenyl-4-chloro-2-butene-HCl (II), m. 163-4° (EtOH). II (10 g.) is agitated with 45 ml. CH₂Cl₂ and 25 ml. 2N NaOH 15 min.; the combined organic solvents give 72% 1,4,6,7-tetrahydro-9,10-dimethoxy-2-phenyl-11bH-benzo[a]quinolizine (III), m. 123-5° (iso-PrOH); HCl salt m. 200-1°; HBr salt m. 214-16°. A solution of 440 mg. III.HCl in 22 ml. MeOH and 1 ml. 2N NaOH is hydrogenated at room temperature under normal pressure in the presence of Raney Ni, the catalyst filtered off, the solvent evaporated, the residue mixed with 5 ml. H₂O and extracted with 4 portions CH₂Cl₂, and the exts. evaporated to give 75% 1,2,3,4,6,7-hexahydro-9,10-dimethoxy-2-phenyl-11bH-benzo[a]quinolizine, m. 89-90° (iso-PrOH); HCl salt m. 229-30°; HBr salt m. 202-4° (decompn). A solution of 60 g. 6,7-dimethoxy-3,4-dihydroisoquinoline in 700 ml. H₂O and 250 ml. MeOH are added to a citrate-buffered aqueous solution (pH 4.6) and mixed with 60 g. of BzCH₂CO₂H in 200 ml. 2 N NaOH, the volume made up to 2 l. with H₂O and MeOH, the mixture kept 20 hrs. at pH 4.6 and 25°, and 250 ml. 2N NaOH added to give 88% 1-phenacyl - 6,7 - dimethoxy - 1,2,3,4 - tetrahydroisoquinoline, m. 138-9° (Me₂CO). The following were similarly prepd: bis[(2-benzoyl-6,7-dimethoxy - 1,2,3,4 - tetrahydro - 1 - isoquinolyl)methyl](1-buten-2-yl)carbinol (IV), m. 225-7° (HCONMe₂-EtOH); bis [(6,7 - dimethoxy - 1,2,3,4 - tetrahydro - 1 - isoquinolyl)methyl] - [1-buten-2-yl]carbinol, m. 126-8° (di-HCl salt m. 250-2°); 1-(6,7-dimethoxy-1,2,3,4-tetrahydro-1-isoquinolyl) - 2 - [(6,7 - dimethoxy-1,2,3,4-tetrahydro-1-isoquinolyl)methyl] - 3- chloromethyl-2-pentene-2HCl, m. 230-3°; α,α'-bis(2- benzoyl-6,7-dimethoxy-1,2,3,4-tetrahydro-1-isoquinolyl)acetone-2HBr, m. 204-5° (meso form m. 178-80°; dibenzoyl derivative m. 198°); bis[(2-benzoyl-6,7-dimethoxy-1,2,3,4-tetrahydro- 1-isoquinolyl)methyl] (1 - buten - 2-yl)carbinol; bis [(6,7-dimethoxy- 1,2,3,4-tetrahydro- 1-isoquinolyl)methyl] (1-buten-2-yl)carbinol; 2-dehydroemetine(3-ethyl-9,10-dimethoxy-1,6,7,11b-tetrahydro-2-[(6,7- dimethoxy - 1,2,3,4- tetrahydro-1-isoquinolyl)methyl]-4H- benzo[a]quinolizine, m. 112-14° and 194-5° (di-HCl salt m. 248-50°); α,α'-bis(N-benzoyl-6,7-dimethoxy-1,2,3,4-tetrahydro-1-isoquinolyl)acetone, m. 178-80°; α,α'-bis (6,7-dimethoxy- 1,2,3,4-tetrahydro-1-isoquinolyl)acetone, m. 144-5° (di-HCl salt m. 193-5°; methanesulfonate m. 173-4°); α,α'-bis(2-acetyl-6,7-dimethoxy-1,2,3,4-tetrahydro-1-isoquinolyl)acetone, m. 191-2°; bis[(6,7-dimethoxy-1,2,3,4- tetrahydro-1-isoquinolyl)methyl]-1-buten-2-ylcarbinol-2HCl, m. 193-201°; 9,10-dimethoxy-1,6,7,11b-tetrahydro-2-heptyl-4H-benzo [a] quinolizidine; 1-phenacyl-2-benzoyl - 6,7 - dimethoxy-1,2,3,4- tetrahydroisoquinoline, m. 190-3°; [(2-benzoyl-6,7-dimethoxy - 1,2,3,4 - tetrahydro - 1 - isoquinolyl)methyl]-(phenyl)(1-buten-2- yl)carbinol, m. 164-6° (AcOH ester); (6,7-dimethoxy-1,2,3,4- tetrahydro-1-isoquinolyl)-3-phenyl-2-ethyl - 1-buten-3-ol-HCl, m. 191-3° (iso-PrOH) [free base m. 115-16° (iso-PrOH-H₂O)]; 1,4,6,7-tetrahydro-9,10-dimethoxy-2-phenyl-3-ethyl-11bH- benzo[a]quinolizine-HCl, m. 209-12° (iso-PrOH) (perchlorate m. 198-9°); 3-ethyl-9,10-diethoxy-1,6,7,11b-tetrahydro-2-[(1,2,3,4- tetrahydro-6,7 - diethoxy - 1 - isoquinolyl)methyl]-4H-benzo [a] quinolizine-2HCl; 3-ethyl-9,10-diethyl-1,6,7,11b-tetrahydro-2-[(1,2,3,4 - tetrahydro - 6,7 - diethyl - 1 - isoquinolyl)-methyl]-4H-benzo[a] quinolizine -2HCl; 1,4,6,7- tetrahydro-2-phenyl-11bH-benzo [a] quinolizine-2HCl; 1,2,3,4,6,7-hexahydro-2-phenyl- 11bH-benzo [a] quinolizine; 1,2,3,4,6,7-hexahydro-9-chloro-2-phenyl- 11bH-benzo[a] quinolizine (V); 3-ethyl-9,10-methylenedioxy - 1,6,7,11b - tetrahydro - 2 - [(1,2,3,4 - tetrahydro-6,7-methylenedioxy - 1 - isoquinolyl)methyl] - 4H - benzo[a] quinolizine; α,α'-bis(2-acetyl-6,7-methylenedioxy- 1,2,3,4-tetrahydro-1-isoquinolyl)acetone-2HBr, m. 243-7° 188-9° (decomposition).

IT 96377-86-5, 1-Isoquinolineethanol, 2-benzoyl-α-(1-ethylvinyl)-1,2,3,4-tetrahydro-6,7-dimethoxy-α-phenyl-
(preparation of)
RN 96377-86-5 HCAPLUS
CN 1-Isoquinolineethanol, 2-benzoyl-α-(1-ethylvinyl)-1,2,3,4-tetrahydro-
6,7-dimethoxy-α-phenyl- (7CI) (CA INDEX NAME)



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=> fil caold

FILE 'CAOLD' ENTERED AT 11:35:54 ON 31 AUG 2004

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FILE COVERS 1907-1966

FILE LAST UPDATED: 01 May 1997 (19970501/UP)

This file contains CAS Registry Numbers for easy and accurate substance identification. Title keywords, authors, patent assignees, and patent information, e.g., patent numbers, are now searchable from 1907-1966. TIFF images of CA abstracts printed between 1907-1966 are available in the PAGE display formats.

This file supports REGISTRY for direct browsing and searching of all substance data from the REGISTRY file. Enter HELP FIRST for more information.

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=> s l24

L26 1 L24

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=> d all l26

L26 ANSWER 1 OF 1 CAOLD COPYRIGHT 2004 ACS on STN

AN CA61:3079h CAOLD

TI 8-aminoquinoline

AU Korzunov, N. P.

DT Patent

TI quinolizine derivs.

AU Schoepf, Clemens; Klug, R.

PA Merck, E., A.-G.

DT Patent

PATENT NO. KIND DATE

PI SU 161757


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PI    US 3132147          1964
      BE 632428
      FR 1431659
      GB 977725
IT    2649-50-5   4914-30-1   21319-81-3   47728-07-4   66833-37-2   94910-05-1
      96269-28-2   96369-40-3   96369-41-4   96377-86-5   96670-94-9
      96706-87-5   97014-12-5   97924-15-7   97924-16-8   97924-37-3   97925-18-3
      98588-30-8   100232-63-1   101057-23-2   101060-09-7   104645-01-4   106401-82-5
      107225-50-3   112001-55-5

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NO ANSWERS SELECTED. THE ANSWER SET WAS CREATED IN FILE 'HCAPLUS'.
USE THE FILE COMMAND TO CHANGE TO THE CORRECT FILE.

=> select hitrn 126

ENTER ANSWER NUMBER OR RANGE (1-):.
'HITRN' IS NOT A VALID FIELD CODE FOR FILE 'CAOLD'
ENTER DISPLAY CODE (IT) OR ?:rn
E1 THROUGH E25 ASSIGNED

=> select hit rn 126

ENTER ANSWER NUMBER OR RANGE (1-):.
E26 THROUGH E26 ASSIGNED

=> fil reg

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STRUCTURE FILE UPDATES: 30 AUG 2004 HIGHEST RN 736108-36-4
DICTIONARY FILE UPDATES: 30 AUG 2004 HIGHEST RN 736108-36-4

TSCA INFORMATION NOW CURRENT THROUGH MAY 21, 2004

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Crossover limits have been increased. See HELP CROSSOVER for details.

Experimental and calculated property data are now available. For more
information enter HELP PROP at an arrow prompt in the file or refer
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<http://www.cas.org/ONLINE/DBSS/registryss.html>

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L27 1 96377-86-5/RN

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L27 ANSWER 1 OF 1 REGISTRY COPYRIGHT 2004 ACS on STN

RN 96377-86-5 REGISTRY

CN 1-Isoquinolineethanol, 2-benzoyl- α -(1-ethylvinyl)-1,2,3,4-tetrahydro-
6,7-dimethoxy- α -phenyl- (7CI) (CA INDEX NAME)

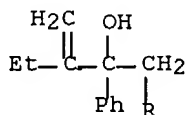
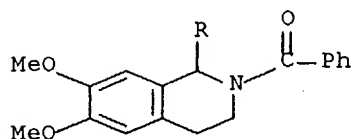
MF C30 H33 N O4

LC STN Files: BEILSTEIN*, CA, CAOLD, CAPLUS

(*File contains numerically searchable property data)

DT.CA Caplus document type: Patent

RL.P Roles from patents: NORL (No role in record)



PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

- 1 REFERENCES IN FILE CA (1907 TO DATE)
- 1 REFERENCES IN FILE CAPLUS (1907 TO DATE)
- 1 REFERENCES IN FILE CAOLD (PRIOR TO 1967)

REFERENCE 1: 61:18195